## 1,3-Dimethyl-4-ethylbenzene 874-41-9 | DTXSID0061246

## Model Performance

|        | n .    |
|--------|--------|
| Model  | I )ata |
| Widdei | Data   |
|        |        |

# Weighted KNN model

| 5-fold CV ( | 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |  |
|-------------|-----------------|------|----------------|------|------------|--|
| Q2          | RMSE            | R2   | RMSE           | R2   | RMSE       |  |
| 0.93        | 22.5            | 0.93 | 22.1           | 0.93 | 22.1       |  |

### Model Results

Predicted value: 188 °C

Global applicability domain: Inside

Local applicability domain index: 7.94e-01

Confidence level: 9.36e-01

## Nearest Neighbors from the Training Set

#### Image not found

1,3-Dimethyl-4-ethylbenzene

Measured: 188 Predicted: 188

#### Image not found

1,3-Dimethyl-5-ethylbenzene

Measured: 184 Predicted: 188

#### Image not found

1,2-Dimethyl-4-ethylbenzene

Measured: 190 Predicted: 188

#### Image not found

2-Ethyl-p-xylene Measured: 187 Predicted: 188

#### Image not found

1-Ethyl-2,3-dimethylbenzene

Measured: 194 Predicted: 188